

Melting of Spherical Yukawa Clusters Analyzed by Monte Carlo Simulation

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We analyze the melting of spherical Yukawa clusters by Monte Carlo simulations. Spherical clusters are expected to be found in dusty plasmas in an isotropic environment such as microgravity and serve as a model for classical clusters. We obtain the specific heat through fluctuations of the potential energy and identify its peak as the transition temperature. Melting temperatures are compared with those of bulk Yukawa systems and it is confirmed that the melting temperature increases and approaches the bulk value with the increase of the system size.

I. INTRODUCTION

Dust particles are often observed in plasmas for plasma processes in manufacturing semiconductors and other materials. Since macroscopic particulates usually deteriorate the quality of products, the analysis of their behavior and their control is an important issue in plasma processes.

On the other hand, dust particles have large negative charges and provide us with a typical example of strongly coupled system. They form themselves into various self-organized structures generally called plasma crystals [1]. These ordered structures are useful in estimating physical quantities related to dust particles and ambient plasmas. There also is a possibility to apply their ordering to device processes.

Dust particles are organized into layered structures in experiments on the ground due to large gravity acting on them. In recent years, experiments under microgravity realized by free fall or in the space station have been performed [2] and attracting attention from the expectation to observe their inherent properties free from the effect of gravity.

We have studied the behavior of the finite system of dust particles regarded as a Yukawa system [3,4]. We have found that they are organized into spherical clusters composed of onion shells and dependence on the parameters of the Yukawa systems has been analyzed.

In this paper, we analyze the melting of the clusters of dust particles by Monte Carlo (MC) simulations. The resultant information may be useful as a probe

for plasma parameters. Since the Yukawa interaction covers both the long-range and the short-range interactions, comparison with the melting of Coulomb and Lennard-Jones clusters will also be useful in understanding those of classical clusters.

II. YUKAWA SYSTEM

We consider a finite system of dusty plasmas with a volume V composed of N_d dust particles, N_i ions, and N_e electrons. The charges of dust particles, ions, and electrons are denoted by $-Qe$, e , and $-e$, respectively. We assume that this system satisfies the charge neutrality condition

$$(-Qe)n_d + en_i + (-e)n_e = 0, \quad (1)$$

where the densities of the components n_α ($\alpha = d, i$ and n) are given by $n_\alpha = N_\alpha/V$.

Taking a statistical average over electron and ion degrees of freedom, we obtain the Yukawa system [3] where dust particles are interacting via Yukawa potential

$$v(r) = \frac{(-Qe)^2}{r} \exp(-r/\lambda) \quad (2)$$

and ions and electrons are regarded as background charges. In the isotropic condition realized under microgravity we may assume electrons and ions uniformly fill a sphere and serve as the source of the confining potential for dust particles. The screening pa-

parameter λ defined by

$$\frac{1}{\lambda^2} = \frac{4\pi n_e e^2}{k_B T_e} + \frac{4\pi n_i e^2}{k_B T_i} \quad (3)$$

represents the strength of screening by ambient plasma of ions and electrons which have temperature T_i and T_e , respectively.

Potential energy U of dust particles is expressed as

$$U = \frac{1}{2} \sum_{i,j(i \neq j)} v(r_{ij}) + \sum_i \phi_{ext}(r_i). \quad (4)$$

Here $\phi_{ext}(r)$ is given by an integral over a volume V filled by ambient plasma of electrons and ions as

$$\phi_{ext}(\mathbf{r}) = -n_d(Qe)^2 \int_V d\mathbf{r}' \frac{\exp(-|\mathbf{r} - \mathbf{r}'|/\lambda)}{|\mathbf{r} - \mathbf{r}'|}. \quad (5)$$

Denoting the radius of the sphere of background charges by R , we have

$$\begin{aligned} \phi_{ext}(r) &= 4\pi n_d(Qe)^2 \lambda^2 \\ &\times \left[1 - \frac{\lambda}{r} \exp\left(\frac{-R}{\lambda}\right) \left(1 + \frac{R}{\lambda}\right) \sinh\left(\frac{r}{\lambda}\right) \right] \end{aligned} \quad (6)$$

for $r \leq R$ and

$$\begin{aligned} \phi_{ext}(r) &= 4\pi n_d(Qe)^2 \lambda^2 \frac{\lambda}{r} \exp\left(\frac{-r}{\lambda}\right) \\ &\times \left[\frac{R}{\lambda} \cosh\left(\frac{R}{\lambda}\right) - \sinh\left(\frac{r}{\lambda}\right) \right] \end{aligned} \quad (7)$$

for $r > R$.

This system is characterized by three dimensionless parameters; the number of dust particles N_d , the strength of coupling

$$\Gamma = \frac{(Qe)^2}{ak_B T}, \quad (8)$$

and

$$\xi = \frac{a}{\lambda}. \quad (9)$$

Here the mean distance of dust particles a is defined by $a = (3/4\pi n_d)^{1/3}$.

III. MONTE CARLO SIMULATION

We perform the standard MC simulations following Metropolis et al. [5] to analyze thermodynamic quantities of Yukawa clusters. We obtain the average and the mean square fluctuation of the potential energy by sampling $10^7 - 10^9$ MC steps at each temperature after equilibration. The specific heat C_v is derived from the fluctuation by

$$C_v = \frac{(\langle U^2 \rangle - \langle U \rangle^2)}{k_B T^2}. \quad (10)$$

In Figs. 1-5, the results for some combinations of parameters are shown. In each pair of the figures, left-hand sides (a) are potential energies and right-hand sides (b) are specific heats given by Eq. (10).

In Figs. 1-5 (a), we see that the slope of the potential energy becomes slightly steep at some temperature. For example, this occurs at $1/\Gamma \sim 2 \times 10^{-3}$ in the case of $N_d = 500$ and $\xi = 1$. These seem to signal the melting of the clusters. The changes in the slopes, however, are not so clear as in the bulk system where the potential energy has a discontinuity.

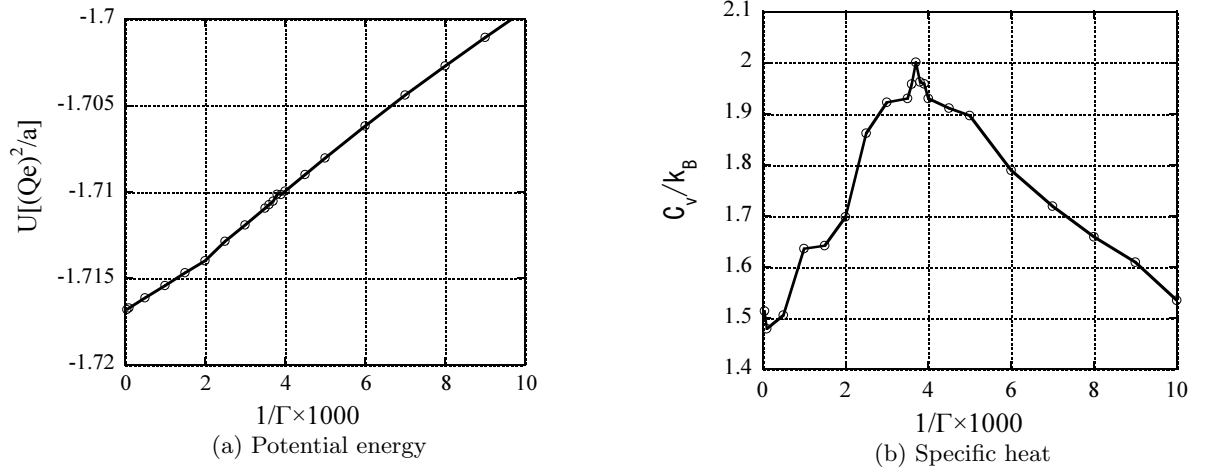
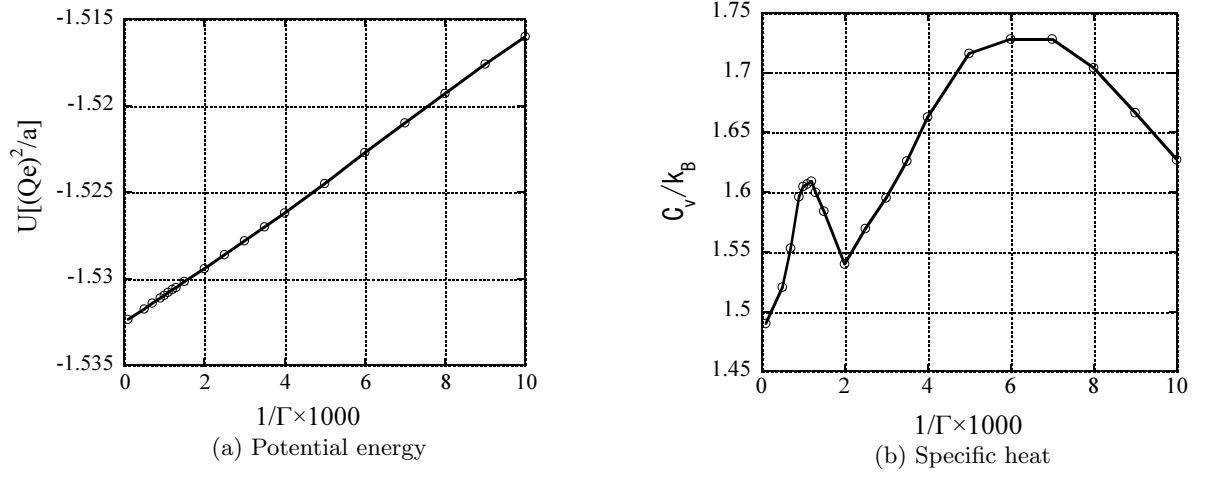
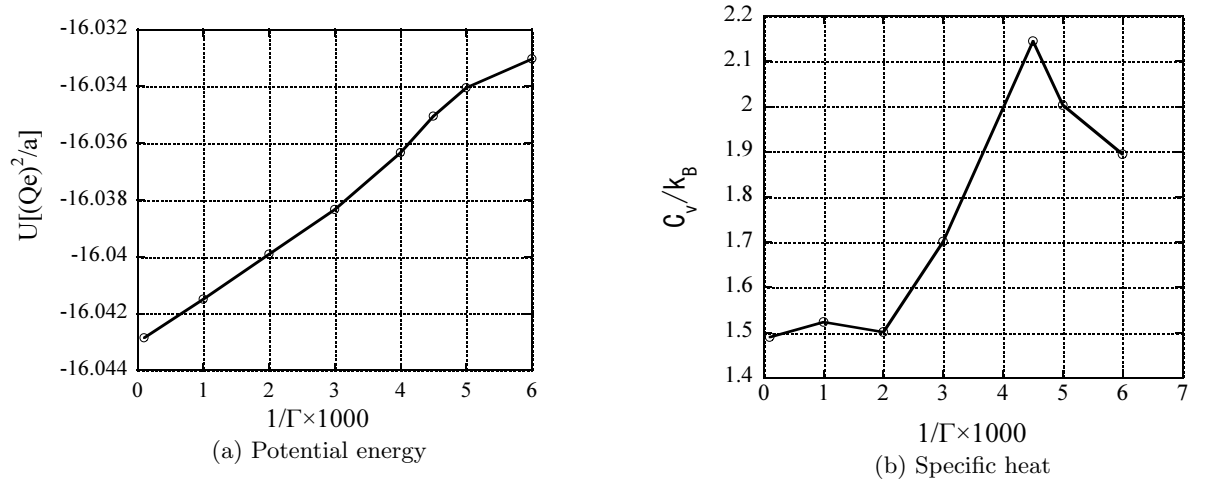
The specific heat in Figs. 1-5 (b) has a well-defined peak, for example, $1/\Gamma \sim 3.7 \times 10^{-3}$ in Fig. 1 (b) for $N_d = 500$ and $\xi = 1$. In the case of $N_d = 100$ and $\xi = 1$ in Fig. 2 (b), the behavior of the specific heat is not simple and has also a broad but higher peak. Considering that the bulk system melts at $1/\Gamma \sim 4.6 \times 10^{-3}$, we may tentatively regard the peak at the lower temperature as a sign of the meltings leaving the nature of broad peak unresolved.

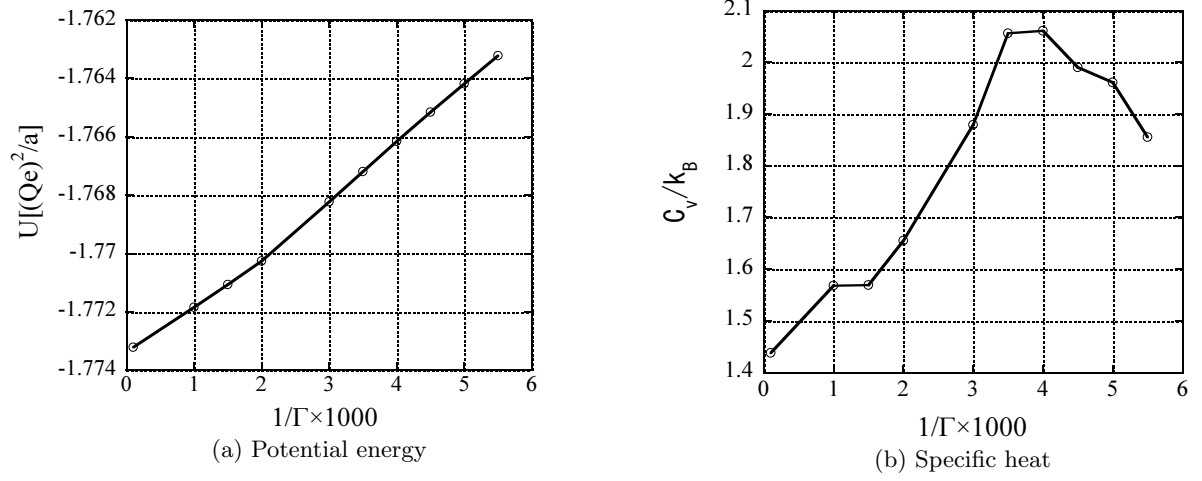
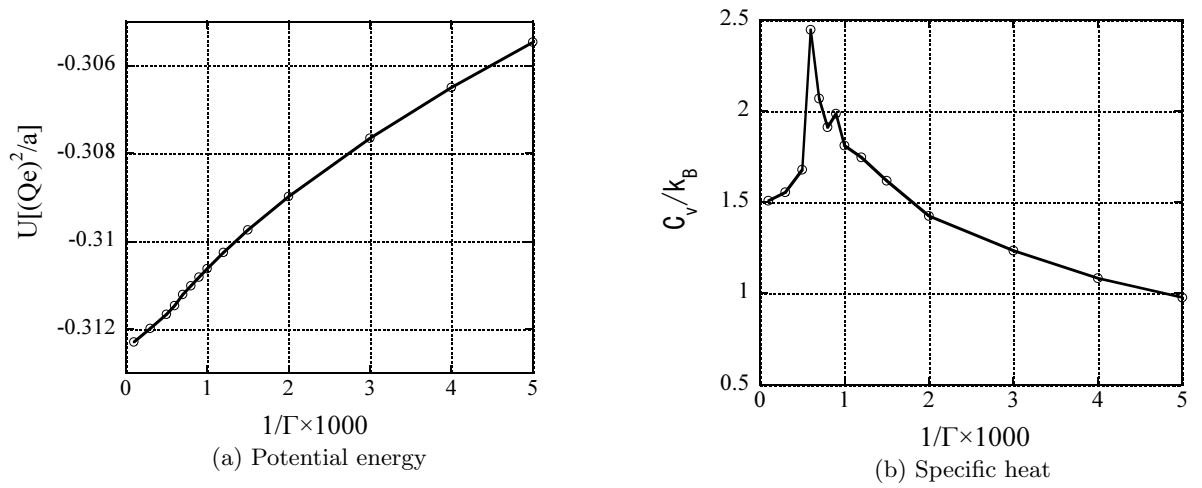
We denote the value of Γ at the melting temperature of clusters by $\Gamma_m(N_d, \xi)$ as a function of N_d and ξ . From Fig. 1 (b), we have $1/\Gamma_m(500, 1) \sim 3.7 \times 10^{-3}$ and the ratio of $1/\Gamma_m(500, 1)$ to the melting temperature of bulk system $1/\Gamma_m(N_d = \infty, 1) = 4.6 \times 10^{-3}$ [6] is 0.80.

We summarize the results of $\Gamma_m(N_d, \xi)$ in Table I. When ξ is fixed (at $\xi = 1$), the value of $1/\Gamma_m$ increases with N_d and approaches the melting temperature of bulk systems. When N_d is fixed (at $N_d = 1000$), $\Gamma_m(N_d, \xi)$ decreases with increase of ξ in accordance with the behavior of $\Gamma_m(N_d = \infty, \xi)$.

TABLE I: Transition temperature for spherical Yukawa cluster in terms of $1/\Gamma_m \times 1000$. Numbers in brackets indicate the ratio to the values for bulk system [6].

ξ	$N_d = \infty$	$N_d = 1000$	$N_d = 500$	$N_d = 100$
0.2	5.7	4.0 ± 1.0 (0.70)	—	1.5 ± 0.1 (0.26)
1	4.6	3.75 ± 0.75 (0.82)	3.7 ± 0.1 (0.80)	1.1 ± 0.2 (0.23)
3	0.84	0.55 ± 0.05 (0.65)	—	0.3 ± 0.01 (0.36)

FIG. 1: Potential energy (a) and specific heat (b) vs. $1/\Gamma$ in the case of $N_d = 500$ and $\xi = 1$.FIG. 2: Potential energy (a) and specific heat (b) vs. $1/\Gamma$ in the case of $N_d = 100$ and $\xi = 1$.FIG. 3: Potential energy (a) and specific heat (b) vs. $1/\Gamma$ in the case of $N_d = 1000$ and $\xi = 0.2$.

FIG. 4: Potential energy (a) and specific heat (b) vs. $1/\Gamma$ in the case of $N_d = 1000$ and $\xi = 1$.FIG. 5: Potential energy (a) and specific heat (b) vs. $1/\Gamma$ in the case of $N_d = 1000$ and $\xi = 3$.

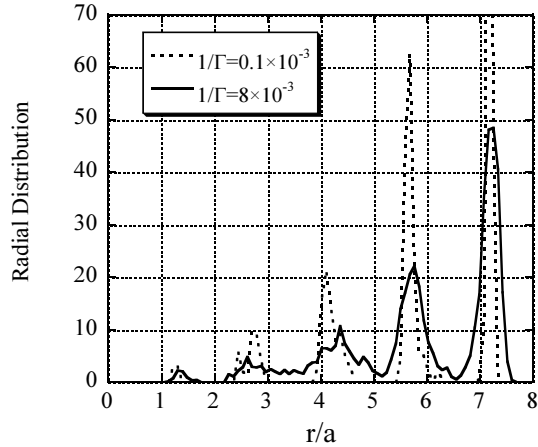


FIG. 6: Radial distribution in the case of $N_d = 500$ and $\xi = 1$.

Radial distributions at $1/\Gamma = 0.1 \times 10^{-3}$ and $1/\Gamma = 8 \times 10^{-3}$ for $N_d = 500$ are shown in Fig. 6. We see that the peaks of the shell structure at $1/\Gamma = 0.1 \times 10^{-3}$ are smeared out at $1/\Gamma = 8 \times 10^{-3}$ especially in the inner part of the cluster. In other words, the most part of

the ordering on the periphery is still left unchanged even at $1/\Gamma = 8 \times 10^{-3}$. This might be the origin of the slowly decaying tail of the specific heat at the high temperature side.

IV. CONCLUSION

We have observed the melting of Yukawa clusters by MC simulations. From the fluctuation in the potential energy, the specific heat is obtained as a function of temperature for some combinations of parameters. The specific heat has a peak structure and when we regard the peak as the transition temperature, the cluster has lower transition temperature than bulk system and the transition temperature increases with the increase of the cluster size approaching the bulk value. In some cases, the structure of the specific heat is not simple as a function of temperature and even broad peaks at temperatures higher than the bulk melting temperature have been found and left unexplained. Molecular dynamics simulations in progress will be helpful to clarify the dynamical nature of melting transition of these clusters.

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